

Hexachloropropene
1888-71-7 | DTXSID7062039

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.67e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.53e-01

Confidence level: 5.48e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Phenyl carbonochloridate</div> <div>Measured: 2.44e-01</div> <div>Predicted: 1.81e-01</div>	<div>Image not found</div> <div>Dimethyl sulfoxide</div> <div>Measured: 2.10e-01</div> <div>Predicted: 3.98e-01</div>	<div>Image not found</div> <div>1-Chloro-2-propanol</div> <div>Measured: 18.5</div> <div>Predicted: 5.24</div>
<div>Image not found</div> <div>2,6-Dichlorophenol</div> <div>Measured: 2.20e-01</div> <div>Predicted: 1.03e-01</div>	<div>Image not found</div> <div>Methyl isothiocyanate</div> <div>Measured: 2.70e-01</div> <div>Predicted: 5.52</div>	